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Heavy-fermion systems

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Abstract : Starting from reminiscences of my stay at Berhampur University during 1974 to 1984, where I did considerable amount of research in a variety of subjects in Condensed Matter Physics, I present a brief review of heavy fermion systems which also includes my work done both at Berhampur and in USA.

Keywords : Heavy fermion systems, Anderson Hamiltonian, Fermi-liquid model, metamagnetism

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1. Introduction

I have been asked to give a brief summary of my research on magnetism at Berhampur University. I started working on magnetism as a PhD student at Tufts University under the supervision of Professor Laura M Roth. The title of my PhD. thesis was "Theory of Diamagnetic Susceptibility of Metals", part of which was published in Physical Review. The main feature was to use the pseudopotential theory of Phillips and Kleinman to derive a theory of diamagnetic susceptibility of metals. This was a significant advancement over Landau's free electron theory. After a brief stint as post-doctoral fellow with Leonard Kleinman at University of Texas at Austin, I joined Utkal University in July 1968 and continued to work on magnetism with my graduate students. In January 1972, I went to University of Texas at Austin for two years as Research Scientist to work again with Professor Kleinman on magnetism. In March 1974, I joined Berhampur University as Professor and Head of Department of Physics. I spent 10.5 years there during which N C Das (Theory of Magnetic Pseudopotentials), S K Misra (Many-Body Theory of Magnetic Susceptibilty of Solids), G S Tripathi (Spin-Orbit and Many-Body effects on Knight Shift), T Sahu (Magnetic Susceptibilty of Tetrahedral Semiconductors), J C Mohanty (Crystal Field Effects and Magnetic Susceptibility of Mixed-Valence Systems), L K Das (Theory of Knight Shift in Metals), N Panigrahi (Magnetic and Dielectric Susceptibilities of Model Amorphous Semiconductors), B Misra (Theory of Knight Shift due to Indirect Nuclear Hyperfine

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Interactions) and S Misra (Theory of Knight Shift in Narrow-Gap Semiconductors) completed their PhD thesis under my supervision. In this brief review of my Berhampur University days, I have listed their publications in the references chronologically (Ref. 1–26) but omitted any of my publications which is neither related to magnetism nor to their work. I have been amazed by the dedication, hard work and zeal with which all of them worked and their confidence in me. In 1995, I went to Berhampur University on a sabbatical and renewed working with G S Tripathi and T Sahu. I am very proud no note that both of them have grown in stature as physicists. Indeed, if I could travel back in time, I would return to Berhampur University, a place my family and I will always cherish and which is now firmly entrenched in the Indian Physics map.

2. Overview of heavy-fermion systems

The heavy-fermion system is a loosely defined collection of intermetallic compounds containing lanthanide (mostly Ce, Yb) or actinide (mostly U, Np) elements. Recently, other compounds such as quasi two-dimensional Ce Co In_5 and 'Skutterdite' $PrOs_4Sb_{12}$ have been shown to exhibit such behavior. I will present an overview of the 'exotic' properties of these systems, the only common feature of which is that they have large effective mass; (50–1000) times greater than the mass of a free electron below a coherence temperature. The effective mass is estimated through the electronic specific heat. The specific heat C_v of a solid can be expressed as

$$Cv / T = \gamma + \delta T^2 , \tag{1}$$

where $\gamma = V_m k_F k_B^2 m^* / 3\hbar^2$, m^* is the effective mass of the electron and T is the absolute temperature. For heavy-fermion systems, γ abruptly increases below the coherence temperature T^*. There is an additional spin-fluctuation term for UPt_3. Some of the other properties of heavy-fermions include (i) an enhanced Pauli spin susceptibility indicating a large effective mass; (ii) the Wilson ratio is approximately one; (iii) a huge T^2 term in the electrical resistivity and (iv) highly temperature-dependent de Haas-van Alphen oscillation-amplitudes at very low temperatures.

The intense interest in heavy-fermion systems started with the discovery of superconductivity in $CeCu_2Si_2$ by Steglich *et al* [27]. The big surprise was that, up to that time, magnetism and superconductivity were considered to be contradictory phenomena. However, in $CeCu_2Si_2$, the 4*f*-electrons which are responsible for local magnetic moments at higher temperatures are also responsible for superconductivity below the critical temperature T_c. After the discovery of high-T_c superconductivity in 1986 and the realization that both high-T_c superconductors and heavy-fermions are not only highly correlated electron systems but also exhibit 'nearness' to magnetism at the superconducting phase, the interest in these systems grew rapidly.

At first it was assumed that while most rare-earth compounds which have either localized 4f-electrons (cerium) or 5-*f* electrons (uranium) are mixed-valence systems, a few become Heavy-Fermions below the coherence temperature. However, it has been discovered that other compounds also exhibit the same properties. At present, approximately fifty heavy-fermion systems have been discovered and there is no uniformity in their properties. Below a certain temperature, some exhibit superconductivity; some others exhibit either ferromagnetism or antiferromagnetism; and several heavy-fermions become semiconductors. Some heavy-fermions are Fermi liquids while some others are non-Fermi liquids. Both magnetic and superconducting quantum critical points have been observed in some of these systems. The only common feature is the large effective mass and the fact that they are highly-correlated electron systems. The wide interest is due to the many unsolved theoretical problems and the wide variety of possible technological applications. The theory of these systems lags behind the experiment although several powerful techniques have been applied. These include Bethe ansatz method, $1/N$ expansion method, renormalization group technique, Dynamical Mean Field theory and Quantum Critical Point. There are several theories for heavy-fermion superconductivity in which there is widespread interest since there is lot of similarities with high-T_c superconductivity. There are a large number of review articles and proceedings of international conferences on heavy-fermions. A few of these (by no means complete) are mentioned in Ref. [28].

3. Exact diagonalization of periodic Anderson model in finite clusters

In the 1980's, it became obvious that the three phenomena of mixed-valence, Kondo, and heavy-fermion behavior, at least in Ce systems, correspond to different regimes of one fundamental phenomenon. In order to correlate these regimes and to study their dependence on the various relevant parameters, we considered the application of the periodic Anderson model to small clusters [29]. The periodic Anderson model relevant to a four-atom cluster (our results for larger clusters are qualitatively similar) with periodic boundary conditions is given by the Hamiltonian

$$\mathcal{H} = t\sum_{i\neq j,\sigma} C^{\dagger}_{j\sigma}C_{j\sigma} + E_f\sum_{i,\sigma} f^{\dagger}_{i,\sigma}f_{i,\sigma} + U\sum_i f^{\dagger}_{i\uparrow}f_{i\uparrow}f^{\dagger}_{i\downarrow}f_{i\downarrow} + V\sum_{i\neq j,\sigma}\left(C^{\dagger}_{i\sigma}f_{j\sigma} + f^{\dagger}_{j\sigma}C_{i\sigma}\right). \quad (2)$$

Here, t is the hopping integral of the extended orthogonal orbitals between sites i and j (restricted to nearest neighbors). $C^{\dagger}_{i\sigma}$ and $C_{i\sigma}$ are the creation and annihilation operators for these extended orbitals with spin σ. There is one extended orbital per spin with a mean energy which is the origin of the energy scale. $f^{\dagger}_{i\sigma}$ and $f_{i\sigma}$ are the creation and annihilation operators for the localized f orbitals with energy E_f. U is the Coulomb repulsion between two electrons of opposite spin in the f orbital and describes a short-range interaction between them. V is a positive hybridization parameter between the localized and the band orbitals in neighboring sites. U is positive while t and f can have either sign. The total number of electrons is one per site. We considered the application to small clusters of four sites of equal length (square, rhombus, and tetrahedron) thereby including the importance of band structure effects. For example, our model Hamiltonian for a tetrahedron is identical to that of an *fcc* lattice if the Brillouin zone sampling is restricted to four reciprocal-lattice points, the zone center τ, and the three square-face-center points X.

The Hamiltonian (2) is conveniently considered on a basis of states diagonal in occupation numbers. We note that spin is a good quantum number and the states can be classified as spin singlets, triplets and quintets. We constructed a computer program to diagonalize the Hamiltonian within subspaces of fixed values of S_z. We have calculated the f-state occupation (n_f), temperature dependence of specific heat (C_v) and the magnetic susceptibility (χ_f) of f-electrons for a large number of parameters. We found that the mixed-valent, Kondo and magnetic regimes depend sensitively on $V/|t|$, and $E_f/|t|$ and the geometry of the clusters but not on U. When $E_f/|t|$ is large and negative, for small values of $V/|t|$ ($n_f \approx 1$), the many-body ground state is nonmagnetic, but the next two excited states are magnetically ordered and nearly degenerate with the ground state. The specific heat rises sharply at low temperatures and the system exhibits heavy-fermion behavior. In some cases, the ground state is magnetically ordered but nearly degenerate with a nonmagnetic excited state and well separated from other states. This corresponds to heavy-fermions with magnetically ordered ground state. In some cases, there is a transition from the Kondo lattice to a magnetic regime and subsequent reentry into either a Kondo-lattice or a mixed-valence regime as E_f is gradually increased from large negative values. We also find that mixed valence and magnetic order can coexist for a very narrow range of E_f for some choice of parameters.

4. Fermi-liquid model for Kondo lattice systems

I present an outline of a Fermi liquid theory for some Kondo lattice systems ($CeCu_2Si_2$, $CeAl_3$ *etc.*) in which spin-orbit effects are specifically included [30]. The ground state of a Kondo ion is a singlet, and a renormalized resonant level (RL) is a good description of the low-energy behavior of such a system. The RL, which is characterized by an effective width Δ^* and an effective f level position E_f^*, describes a renormalized f state with $2J + 1 = N$ scattering channels, each with a azimuthal quantum number m_j. For a Kondo lattice, the scattering at each Kondo site can be described by a phase shift

$$\delta_\nu(\varepsilon) = \delta(\mu) + (\varepsilon - \mu)/T_K + \sum_{\nu'\varepsilon'} \varphi_{\nu\nu'} \delta n_{\nu'}(\varepsilon'), \tag{3}$$

where ν and ν' denote the spin-orbital states of the localized f level, T_K is the Kondo temperature and $\delta(\mu)$ is fixed by the valence of the Kondo ion and by using the Friedel sum rule. Requiring that the scattering of the lattice at $T = 0$ ($\delta n_{\nu'} = 0$) is coherent leads to the KKRZ equations whose solutions near ν, E_K, correspond to energies of single quasi-particle excitations. Two quasi-particles interact when one 'senses' the virtual polarization of a Kondo ion induced by another. This interaction is characterized by the parameters $\varphi_{\nu\nu'}$. In cerium systems, only the $l = 3$ phase shift is important. The spin-orbit splitting between $J = 5/2$ and $7/2$ is much larger than Δ^*, and therefore $\delta_3(\varepsilon)$ is large in the $J = 5/2$ state. It is easy to show, by using a procedure similar to the KKRZ method and including spin-orbit effects, that the band structure is obtained from

$$\det\left\|\left(k_n^2 - E\right)\delta_{kns,\,kn's'} + \Gamma_{kns,\,kn's'}\right\| = 0, \tag{4}$$

where Γ is a complicated function [30] of Bessel functions, Clebsch-Gordon coefficients and spherical harmonics. After considerable algebra, we obtain the secular equations of a hybridization Hamiltonian

$$\mathcal{H} = \sum_{k,n,s}\varepsilon_n(k)C^\dagger_{kns}C_{kns} + \sum_{k,s,J}E_{fJ}f^\dagger_{ksJ}f_{ksJ} + \sum_{k,n,s,s',J}\gamma^J_{ks,kns'}(f^\dagger_{ksJ}C_{kns'} + C^\dagger_{kns'}f_{knJ}). \tag{5}$$

Here, $\varepsilon_n(k)$ is the energy of the n-th Brillouin zone obtained by diagonalizing the Hamiltonian containing the kinetic energy term and the corresponding spin-orbit pseudopotential term (including l = 3), $\gamma^J_{ks,kn,s'}$ are the hybridization potentials derived by us [30] and C_{kns} ($C^\dagger_{kns}$); f_{ksJ} ($f^\dagger_{ksJ}$) are the usual fermion operators. The energy E_{fJ} is dispersionless but the hybridization term mixes the localized states with the extended states of all Brillouin zones. The Hamiltonian (5) can be transformed into one with one extended band only by a projection method suggested by Heine. If this procedure is adopted, one obtains the hybridization of one conduction band with localized states which have dispersion in their energy and one obtains a periodic Anderson Hamiltonian in which spin-orbit effects are explicitly included.

We have used degenerate perturbation theory to construct Bloch functions which are eigenfunctions of the Hamiltonian in eq. (4). We have used these functions to evaluate the momentum and spin matrix elements which occur in the general expressions for spin magnetic susceptibility (χ_s) of Misra *et al.* and for Knight shift (K_s) of Tripathi *et al.* and shown that K_s is not directly proportional to χ_s, a result which is well known for Kondo-lattice systems.

5. Metamagnetism and paramagnetism in heavy-fermions

A high magnetic field can either suppress antiferromagnetism or induce 'metamagnetism'. Metamagnetism, which manifests macroscopically in an abrupt increase of the bulk magnetization at a critical field (H_c), has been widely studied in both itinerant systems as well as in some heavy fermions (*i.e.*, $CeRu_2Si_2$, UPt_3 and $Sr_3Ru_2O_7$). The metamagnetic transition, which is associated with a hysteresis in the magnetization curve, disappears at high temperature. We consider a variant of the periodic Anderson Hamiltonian in the momentum-space representation in an applied magnetic field $\boldsymbol{H}$ [31]

$$\begin{aligned}\mathcal{H} = {} & \sum_{k\sigma}\varepsilon_{ck}C^\dagger_{k\sigma}C_{k\sigma} + U_c\sum_{kk'q}C^\dagger_{k+q\uparrow}C_{k\uparrow}C^\dagger_{k'-q\downarrow}C_{k'\downarrow} + \sum_{k\sigma}\varepsilon_{fk}f^\dagger_{k\sigma}f_{k\sigma} \\ & + U_f\sum_{kk'q}f^\dagger_{k+q\uparrow}f_{k\uparrow}f^\dagger_{k'-q\downarrow}f_{k'\downarrow} + \sum_{k\sigma}V_{k\sigma}\left(C^\dagger_{k\sigma}f_{k\sigma} + f^\dagger_{k\sigma}C_{k\sigma}\right) \\ & + \mu_B\sum_k\Big\{H_z\left(C^\dagger_{k\uparrow}C_{k\uparrow} - C^\dagger_{k\downarrow}C_{k\downarrow} + f^\dagger_{k\uparrow}f_{k\uparrow} - f^\dagger_{k\downarrow}f_{k\downarrow}\right) \\ & + \left[\left(C^\dagger_{k\uparrow}C_{k\downarrow} + f^\dagger_{k\uparrow}f_{k\downarrow}\right)H_+ + \left(C^\dagger_{k\downarrow}C_{k\uparrow} + f^\dagger_{k\downarrow}f_{k\uparrow}\right)H_-\right]\Big\}.\end{aligned} \tag{6}$$

All these terms are explained in Ref. [31]. The Hamiltonian has been written in this form since we wish to explain metamagnetism based on spin fluctuations (caused by the transverse components of the magnetic field H_+ and H_-) and their damping in the high field state. We have used a mean field approximation (MFA) for the electron correlation energies. For the high field magnetic state, we have derived equations of motion for the magnetization and spin-fluctuation amplitudes using Heisenberg's equation. Spin fluctuation and magnetization dampings are considered phenomenologically. Metamagnetism is shown to be driven by the transverse part of the applied field and strong electron-electron correlations are found to be important in the high field state.

We now analyze the low field paramagnetic susceptibility in the limit of $H_z \to 0$, in the presence of many body and conduction electron moment and local moment interactions, the one-electron Green's function satisfies the equation [31]

$$(\zeta_1 - \mathcal{H})G(\boldsymbol{r}, \boldsymbol{r}', H_z, \mu_z, \zeta_1) = \delta(\boldsymbol{r} - \boldsymbol{r}'), \tag{7}$$

where $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{s-f} + \mathcal{H}_{Hz} + \sum(\boldsymbol{r}, \boldsymbol{r}', H_z, \mu_z, \zeta_1)$. (8)

The details of our numerical calculations for $CeRu_2Si_2$ are explained in Ref. [31]. The *m vs. h* curve Ref. [31] shows hysterisis behavior, *i.e.* there are two critical fields of metamagnetic transition (h_m) at 5.8 and 6.6 T. The average 6.2 T is not very different from the experimental value of 7.8 T. The average jump in the magnetization is 0.68 μ_B as compared to the predicted experimental value of 0.5 μ_B. The slope of *m vs. h* curve is steeper for $h<h_m$ compared to $h>h_m$. Which is also in agreement with experimental observation. Thus, most of the systematics observed in case of metamagnetic transition are explained by our model qualitatively.

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